

# Transitions between the $4f$ -core-excited states in $\text{Ir}^{16+}$ , $\text{Ir}^{17+}$ , and $\text{Ir}^{18+}$ ions for clock applications

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Iridium ions near  $4f$ - $5s$  level crossings are the leading candidates for a new type of atomic clocks with a high projected accuracy and a very high sensitivity to the temporal variation of the fine structure constant  $\alpha$ . To identify spectra of these ions in experiment accurate calculations of the spectra and electromagnetic transition probabilities should be performed. Properties of the  $4f$ -core-excited states in  $\text{Ir}^{16+}$ ,  $\text{Ir}^{17+}$ , and  $\text{Ir}^{18+}$  ions are evaluated using relativistic many-body perturbation theory and Hartree-Fock-Relativistic method (COWAN code). We evaluate excitation energies, wavelengths, oscillator strengths, and transition rates. Our large-scale calculations includes the following set of configurations:  $4f^{14-k}5s^m5p^n$  with  $(k+m+n)$  equal to 3, 2, and 1 for the  $\text{Ir}^{16+}$ ,  $\text{Ir}^{17+}$ , and  $\text{Ir}^{18+}$  ions, respectively. The  $5s-5p$  transitions are illustrated by the synthetic spectra in the 180 - 200 Å range. Large contributions of magnetic-dipole transitions to lifetimes of low-lying states in the region below 2.5 Ry are demonstrated.

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## I. INTRODUCTION

Selected transitions involving electron holes, i.e. vacancies in otherwise filled shells of atomic systems in highly-charged ions were shown to have frequencies within the range of optical atomic clocks, have small systematic errors in the frequency measurements and be highly sensitive to the temporal variation of the fine structure constant  $\alpha$  [1]. Sympathetic cooling of highly-charged ions has been demonstrated in [2].

This work is motivated by these applications of highly-charged ions and recent experimental work including identification of M1 transitions in  $\text{Ir}^{17+}$  spectra [2–4]. In 2015, identification of the predicted  $5s-4f$  level crossing optical transitions was presented by Windberger *et al.* [3]. The spectra of Nd-like W, Re, Os, Ir, and Pt ions of particular interest for tests of fine-structure constant variation were explored [3]. The authors exploited characteristic energy scalings to identify the strongest lines, confirmed the predicted  $5s-4f$  level crossing, and benchmarked advanced calculations.

In the present work, we have employed Hartree-Fock-Relativistic method (COWAN code) and relativistic many-body perturbation theory (RMBPT) to study  $\text{Ir}^{16+}$ ,  $\text{Ir}^{17+}$ , and  $\text{Ir}^{18+}$  ions. Excitation energies, wavelengths, transition rates, energies of the lower and upper level, lifetimes, and branching ratios from M1 and E1 transitions in Nd-, Pm-, and Pr-like Ir ions are evaluated. We have used our results to construct synthetic spectra for all three ions. Our goal was to also to investigate the general structure and level distributions in these ions.

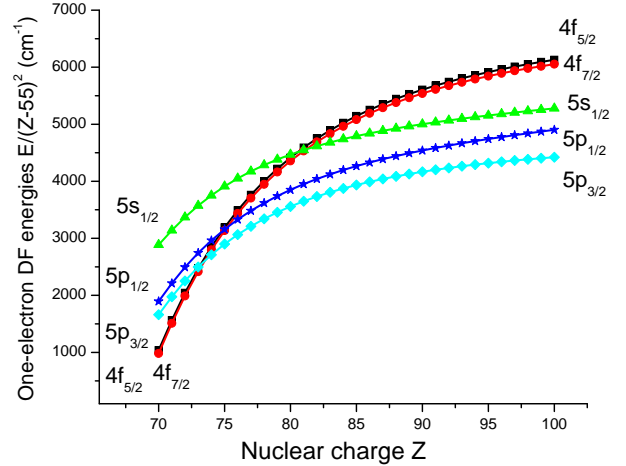


FIG. 1: Dirac-Fock binding energies of the  $4f$ ,  $5s$ , and  $5p$  orbitals as a function of  $Z$  in Er-like ions. Er is a rare earth element with  $Z = 68$ .

For example, we find that in the case of  $\text{Ir}^{18+}$  ion, the energies of the  $4f^{13}$ ,  $4f^{12}5s$ , and  $4f^{11}5s^2$  configurations are within a relatively small interval below  $274768 \text{ cm}^{-1}$ . The first level with  $5p$  electron,  $4f^{12}5p$  ( $^3H$ ) $^4G_{11/2}$ , lies substantially higher, at  $387658 \text{ cm}^{-1}$  which significantly affects the lifetimes of the lower states.

We also employed RMBPT method for simpler one-particle,  $4f^{14}nl$ , and particle-hole configurations of Ir ions to compare with HFR results.

TABLE I: Energies (in 1000 cm<sup>-1</sup>) in Pm-like Ir<sup>16+</sup>, Nd-like Ir<sup>17+</sup>, and Pr-like Ir<sup>18+</sup> ions given relative to the 4f<sup>13</sup>5s<sup>2</sup> 2F<sub>7/2</sub>, 4f<sup>13</sup>5s 3F<sub>4</sub>, and 4f<sup>13</sup> 2F<sub>7/2</sub> ground states, respectively.

Conf.	Level	Energy	Conf.	Level	Energy	Conf.	Level	Energy
Pm-like Ir <sup>16+</sup> ion			Nd-like Ir <sup>17+</sup> ion			Pr-like Ir <sup>18+</sup> ion		
4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>7/2</sub>	0.000	4f <sup>13</sup> 5s	( <sup>2</sup> F) <sup>3</sup> F <sub>4</sub>	0.000	4f <sup>13</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>7/2</sub>	0.000
4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>5/2</sub>	25.909	4f <sup>13</sup> 5s	( <sup>2</sup> F) <sup>3</sup> F <sub>3</sub>	4.236	4f <sup>13</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>5/2</sub>	26.442
4f <sup>14</sup> 5s	( <sup>1</sup> S) <sup>2</sup> S <sub>1/2</sub>	28.350	4f <sup>14</sup>	( <sup>1</sup> S) <sup>1</sup> S <sub>0</sub>	5.091	4f <sup>12</sup> 5s	( <sup>3</sup> H) <sup>4</sup> H <sub>13/2</sub>	60.142
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> D <sub>7/2</sub>	267.942	4f <sup>13</sup> 5s	( <sup>2</sup> F) <sup>3</sup> F <sub>2</sub>	26.174	4f <sup>12</sup> 5s	( <sup>3</sup> H) <sup>4</sup> H <sub>11/2</sub>	67.687
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> G <sub>11/2</sub>	276.214	4f <sup>13</sup> 5s	( <sup>2</sup> F) <sup>1</sup> F <sub>3</sub>	30.606	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>4</sup> F <sub>9/2</sub>	70.096
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>2</sup> I <sub>13/2</sub>	280.511	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> H) <sup>3</sup> H <sub>6</sub>	33.856	4f <sup>12</sup> 5s	( <sup>1</sup> G) <sup>2</sup> G <sub>7/2</sub>	74.664
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> F) <sup>4</sup> D <sub>7/2</sub>	285.301	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> F) <sup>3</sup> F <sub>4</sub>	42.199	4f <sup>12</sup> 5s	( <sup>3</sup> H) <sup>4</sup> H <sub>9/2</sub>	87.749
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> D <sub>7/2</sub>	286.286	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> H) <sup>3</sup> H <sub>5</sub>	58.261	4f <sup>12</sup> 5s	( <sup>3</sup> H) <sup>2</sup> H <sub>11/2</sub>	89.859
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>1</sup> G) <sup>2</sup> H <sub>9/2</sub>	287.909	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> F) <sup>3</sup> F <sub>2</sub>	63.696	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>4</sup> F <sub>3/2</sub>	92.406
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> G <sub>9/2</sub>	288.623	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> H) <sup>3</sup> H <sub>4</sub>	66.296	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>4</sup> F <sub>5/2</sub>	92.940
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> F <sub>5/2</sub>	289.959	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> F) <sup>3</sup> F <sub>3</sub>	68.886	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>4</sup> F <sub>7/2</sub>	94.508
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> G <sub>5/2</sub>	297.128	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> H) <sup>3</sup> H <sub>4</sub>	89.455	4f <sup>12</sup> 5s	( <sup>1</sup> G) <sup>2</sup> G <sub>9/2</sub>	98.486
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> I <sub>11/2</sub>	303.063	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> P) <sup>3</sup> P <sub>2</sub>	91.765	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>2</sup> F <sub>7/2</sub>	101.805
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> G <sub>9/2</sub>	303.664	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> P) <sup>3</sup> P <sub>0</sub>	101.073	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>2</sup> F <sub>5/2</sub>	102.646
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>1</sup> D) <sup>2</sup> D <sub>3/2</sub>	307.339	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>1</sup> I) <sup>1</sup> I <sub>6</sub>	101.537	4f <sup>12</sup> 5s	( <sup>1</sup> G) <sup>2</sup> G <sub>7/2</sub>	119.089
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> F) <sup>4</sup> G <sub>5/2</sub>	307.948	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>3</sup> P) <sup>3</sup> P <sub>1</sub>	107.843	4f <sup>12</sup> 5s	( <sup>3</sup> P) <sup>4</sup> P <sub>5/2</sub>	122.306
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> F) <sup>4</sup> G <sub>7/2</sub>	309.803	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>1</sup> D) <sup>1</sup> D <sub>2</sub>	117.322	4f <sup>12</sup> 5s	( <sup>3</sup> H) <sup>2</sup> H <sub>9/2</sub>	123.040
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> I <sub>9/2</sub>	312.724	4f <sup>12</sup> 5s <sup>2</sup>	( <sup>1</sup> S) <sup>1</sup> S <sub>0</sub>	178.055	4f <sup>12</sup> 5s	( <sup>3</sup> F) <sup>4</sup> F <sub>3/2</sub>	123.434
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> F) <sup>4</sup> F <sub>5/2</sub>	313.871	4f <sup>12</sup> 5s5p	( <sup>3</sup> H) <sup>5</sup> G <sub>6</sub>	312.027	4f <sup>12</sup> 5s	( <sup>3</sup> P) <sup>4</sup> P <sub>1/2</sub>	129.563
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>2</sup> D <sub>5/2</sub>	315.471	4f <sup>13</sup> 5p	( <sup>2</sup> F) <sup>3</sup> D <sub>3</sub>	319.802	4f <sup>12</sup> 5s	( <sup>1</sup> I) <sup>2</sup> I <sub>13/2</sub>	132.511
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>2</sup> G <sub>7/2</sub>	317.004	4f <sup>12</sup> 5s5p	( <sup>3</sup> F) <sup>5</sup> D <sub>4</sub>	321.722	4f <sup>12</sup> 5s	( <sup>1</sup> I) <sup>2</sup> I <sub>11/2</sub>	132.716
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> F) <sup>4</sup> G <sub>7/2</sub>	317.387	4f <sup>13</sup> 5p	( <sup>2</sup> F) <sup>3</sup> G <sub>4</sub>	322.623	4f <sup>12</sup> 5s	( <sup>3</sup> P) <sup>4</sup> P <sub>3/2</sub>	136.659
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> F <sub>3/2</sub>	319.123	4f <sup>12</sup> 5s5p	( <sup>3</sup> H) <sup>3</sup> I <sub>7</sub>	333.465	4f <sup>12</sup> 5s	( <sup>3</sup> P) <sup>2</sup> P <sub>1/2</sub>	145.476
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> I <sub>9/2</sub>	332.682	4f <sup>12</sup> 5s5p	( <sup>3</sup> H) <sup>5</sup> G <sub>5</sub>	333.531	4f <sup>12</sup> 5s	( <sup>1</sup> D) <sup>2</sup> D <sub>5/2</sub>	147.492
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> P) <sup>4</sup> P <sub>3/2</sub>	335.326	4f <sup>12</sup> 5s5p	( <sup>3</sup> H) <sup>5</sup> G <sub>6</sub>	333.649	4f <sup>12</sup> 5s	( <sup>3</sup> P) <sup>2</sup> P <sub>3/2</sub>	152.098
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> F) <sup>4</sup> G <sub>5/2</sub>	337.196	4f <sup>12</sup> 5s5p	( <sup>3</sup> H) <sup>5</sup> I <sub>5</sub>	340.286	4f <sup>11</sup> 5s <sup>2</sup>	( <sup>4</sup> I) <sup>4</sup> I <sub>15/2</sub>	179.577
4f <sup>14</sup> 5p	( <sup>1</sup> S) <sup>2</sup> P <sub>1/2</sub>	337.757	4f <sup>12</sup> 5s5p	( <sup>1</sup> G) <sup>3</sup> H <sub>4</sub>	342.157	4f <sup>11</sup> 5s <sup>2</sup>	( <sup>4</sup> F) <sup>4</sup> F <sub>9/2</sub>	201.648

The values for low-lying levels are presented in the paper, much more extensive set of results is given in the Supplemental Material [5].

## II. LEVEL CROSSINGS AND 4f ELECTRONS IN HIGHLY-CHARGE IONS

Detailed investigation of level crossings relevant to the design of optical atomic clocks with highly-charged ions and search for  $\alpha$ -variation has been carried out in [6]. Ir ions have been considered in [1]. Below, we discuss level crossings in ions similar to the ones studies in this work.

Correlation and relativistic effects for the 4f – *nl* and 5p – *nl* multipole transitions in Er-like tungsten were investigated in Ref. [7]. Wavelengths, transition rates, and line strengths were calculated for the multipole (E1, M1, E2, M2, and E3) transitions between the excited [Cd]4f<sup>13</sup>5p<sup>6</sup>*nl*, [Cd]4f<sup>14</sup>5p<sup>5</sup>*nl* configurations and the ground [Cd]4f<sup>14</sup>5p<sup>6</sup> state in Er-like W<sup>6+</sup> ion ([Cd]=[Kr]4d<sup>10</sup>5s<sup>2</sup>) using the relativistic many-body perturbation theory, including the Breit interaction.

The binding energies of the 4f, 5p, and 5s orbitals in Er-like ions [7] calculated in Dirac-Fock approximation as function of nuclear charge *Z* are plotted in Fig. 1. For

better presentation, we scaled the energies with a factor of  $(Z-55)^2$ . We find that the 4f orbitals are more tightly bound than the 5p and 5s orbitals at low stages of ionization, while the 5p and 5s orbitals are more tightly bound than the 4f orbitals for highly ionized cases. This leads to crossing of 4f and 5s and 5p levels for some *Z* leading to interesting cases of optical or near-optical transitions in selected highly-charged ions. Large cancellation in binding energy values near the crossing (near *Z* = 74 in the example of Fig. 1) make accurate calculations of transition energies and line strengths very difficult [7].

In Ref. [8], Safronova *et al.* reported results of *ab initio* calculation of excitation energies, oscillator strengths, transition probabilities, and lifetimes in Sm-like ions with nuclear charge *Z* ranging from 74 to 100. Sm has *Z* = 62. One of the unique atomic properties of the samarium isoelectronic sequence is that the ground state changes nine times starting from the [Kr]4d<sup>10</sup>5s<sup>2</sup>5p<sup>6</sup>4f<sup>6</sup>6s<sup>2</sup> <sup>1</sup>S<sub>0</sub> level for neutral samarium, Sm I, and ending with the [Kr]4d<sup>10</sup>4f<sup>14</sup>5s<sup>2</sup> <sup>1</sup>S<sub>0</sub> level for 12 times ionized tungsten, W<sup>12+</sup> [9].

Contributions of the 4f-core-excited states in determination of atomic properties in the promethium isoelectronic sequence with *Z* = 74 – 92 were discussed in Ref. [10]. Excitation energies, transition rates, and life-

TABLE II: Wavelengths ( $\lambda$  in Å), weighted oscillator strengths (gf), weighted transition rates ( $gA_r$  in 1/s) for transitions in Pm-like Ir<sup>16+</sup>, Nd-like Ir<sup>17+</sup>, and Pr-like Ir<sup>18+</sup> ions.

Conf.	Level	Conf.	Level	$\lambda$ in Å	gf	$gA_r$ in 1/s
$4f^{12}5s^25p - 4f^{12}5s5p^2$ transitions in Pm-like Ir <sup>16+</sup> ion						
$4f^{12}5s^25p$	$(^1I)^2K_{15/2}$	$4f^{12}5s5p^2$	$(^1I)^2K_{15/2}^a$	187.3222	12.1796	2.315[12]
$4f^{12}5s^25p$	$(^3H)^4I_{15/2}$	$4f^{12}5s5p^2$	$(^3H)^4I_{15/2}^a$	188.4095	7.6206	1.432[12]
$4f^{12}5s^25p$	$(^3H)^4I_{13/2}$	$4f^{12}5s5p^2$	$(^3H)^4I_{13/2}^b$	189.4141	10.2303	1.902[12]
$4f^{12}5s^25p$	$(^1I)^2H_{11/2}$	$4f^{12}5s5p^2$	$(^1I)^2H_{11/2}^a$	190.2284	7.7758	1.433[12]
$4f^{12}5s^25p$	$(^1G)^2H_{11/2}$	$4f^{12}5s5p^2$	$(^3H)^2I_{11/2}^b$	190.2870	7.6461	1.408[12]
$4f^{12}5s^25p$	$(^1I)^2K_{13/2}$	$4f^{12}5s5p^2$	$(^1I)^2K_{13/2}^a$	190.5154	9.7403	1.790[12]
$4f^{12}5s^25p$	$(^1I)^2I_{13/2}$	$4f^{12}5s5p^2$	$(^1I)^2H_{11/2}^a$	191.9017	6.8966	1.249[12]
$4f^{12}5s^25p$	$(^1D)^2F_{7/2}$	$4f^{12}5s5p^2$	$(^1D)^2F_{7/2}^a$	192.6116	5.6848	1.022[12]
$4f^{12}5s^25p$	$(^3H)^4G_{11/2}$	$4f^{12}5s5p^2$	$(^3H)^4G_{11/2}^b$	192.9081	5.5967	1.003[12]
$4f^{12}5s^25p$	$(^3H)^4I_{11/2}$	$4f^{12}5s5p^2$	$(^3H)^2I_{11/2}^b$	193.3102	7.1596	1.278[12]
$4f^{12}5s^2 - 4f^{12}5s5p$ and $4f^{12}5s5p - 4f^{12}5p^2$ transitions in Nd-like Ir <sup>17+</sup> ion						
$4f^{12}5s5p$	$(^1I)^3K_8$	$4f^{12}5p^2$	$(^1I)^3K_8$	186.9139	5.5800	1.065[12]
$4f^{12}5s^2$	$(^1I)^1I_6$	$4f^{12}5s5p$	$(^1I)^1I_6$	187.4003	8.8646	1.684[12]
$4f^{12}5s^2$	$(^3H)^3H_6$	$4f^{12}5s5p$	$(^3H)^3H_6^b$	190.4460	7.6415	1.405[12]
$4f^{12}5s^2$	$(^3H)^3H_4$	$4f^{12}5s5p$	$(^3H)^3H_4^b$	191.2123	5.6115	1.024[12]
$4f^{12}5s^2$	$(^3H)^3H_5$	$4f^{12}5s5p$	$(^3H)^3I_6^b$	194.1681	7.6418	1.352[12]
$4f^{12}5s^2$	$(^3H)^3H_6$	$4f^{12}5s5p$	$(^3H)^3I_7^a$	194.6655	9.2353	1.625[12]
$4f^{12}5s^2$	$(^1I)^1I_6$	$4f^{12}5s5p$	$(^1I)^1K_7$	195.6155	8.9236	1.555[12]
$4f^{12}5s5p$	$(^1I)^1I_6$	$4f^{12}5p^2$	$(^1I)^1I_6^b$	201.1890	7.8226	1.289[12]
$4f^{12}5s5p$	$(^1I)^1K_7$	$4f^{12}5p^2$	$(^1I)^3K_8$	213.6590	6.9882	1.021[12]
$4f^{11}5s^2 - 4f^{11}5s5p$ transitions in Pr-like Ir <sup>18+</sup> ion						
$4f^{11}5s^2$	$(^2F)^2F_{7/2}^1$	$4f^{11}5s5p$	$(^2F)^2F_{7/2}^1$	182.4907	5.6811	1.138[12]
$4f^{11}5s^2$	$(^2L)^2L_{15/2}$	$4f^{11}5s5p$	$(^2L)^2L_{15/2}^b$	184.2146	11.5687	2.274[12]
$4f^{11}5s^2$	$(^2L)^2L_{17/2}$	$4f^{11}5s5p$	$(^2L)^2L_{17/2}^b$	184.3734	8.2009	1.609[12]
$4f^{11}5s^2$	$(^2I)^2I_{13/2}$	$4f^{11}5s5p$	$(^2I)^2I_{13/2}^b$	186.7641	7.6961	1.472[12]
$4f^{11}5s^2$	$(^2G)^2G_{7/2}^2$	$4f^{11}5s5p$	$(^2G)^2H_{9/2}^2$	187.6959	5.6285	1.066[12]
$4f^{11}5s^2$	$(^4I)^4I_{15/2}$	$4f^{11}5s5p$	$(^4I)^4I_{15/2}^b$	187.7941	10.0169	1.894[12]
$4f^{11}5s^2$	$(^4I)^4I_{13/2}$	$4f^{11}5s5p$	$(^4I)^4I_{13/2}^b$	187.9089	7.4924	1.415[12]
$4f^{11}5s^2$	$(^2H)^2H_{9/2}^2$	$4f^{11}5s5p$	$(^2H)^2I_{11/2}^2$	188.0677	6.8954	1.300[12]
$4f^{11}5s^2$	$(^2H)^2H_{11/2}^1$	$4f^{11}5s5p$	$(^2I)^2K_{13/2}^b$	188.1826	6.6946	1.261[12]
$4f^{11}5s^2$	$(^4I)^4I_{11/2}$	$4f^{11}5s5p$	$(^4I)^4I_{11/2}^b$	188.3409	6.1020	1.147[12]
$4f^{11}5s^2$	$(^4G)^4G_{9/2}$	$4f^{11}5s5p$	$(^4I)^4K_{11/2}^b$	188.5680	5.3585	1.005[12]

times in Pm-like tungsten were evaluated for a large number of states. The ground state for the Pm-like W<sup>13+</sup>, Re<sup>14+</sup>, Os<sup>15+</sup>, and Ir<sup>16+</sup> is  $4f^{13}5s^2\ ^2F_{7/2}$ . For the next Pm-like ion, Pt<sup>17+</sup>, the  $4f^{14}5s\ ^2S_{1/2}$  state becomes the ground state and continues to be the ground state for higher  $Z$  because of the  $4f - 5s$  level crossing

### III. ENERGY LEVELS

Our HFR calculations include the following set of configurations:

- Ir<sup>16+</sup>:  $4f^{14}5s$ ,  $4f^{14}5p$ ,  $4f^{13}5s^2$ ,  $4f^{13}5p^2$ ,  $4f^{13}5s5p$ ,  $4f^{12}5s^25p$ , and  $4f^{12}5s5p^2$ .
- Ir<sup>17+</sup>:  $4f^{14}$ ,  $4f^{13}5s$ ,  $4f^{13}5p$ ,  $4f^{12}5s^2$ ,  $4f^{12}5s5p$ , and  $4f^{12}5p^2$ .
- Ir<sup>18+</sup>:  $4f^{13}$ ,  $4f^{12}5s$ ,  $4f^{12}5p$ ,  $4f^{11}5s^2$ , and

$4f^{11}5s5p$ .

In Table I, we list the limited number of excitation energies in three iridium ions of interest. The energies are given in 1000 cm<sup>-1</sup>. The superscripts  $a$  and  $b$  in this and following tables are seniority numbers used to distinguish levels that have the same electronic configurations, intermediate and final terms. We note that the energy differences between the doublet  $4f^{13}5s^2\ ^2F_J$  levels and the  $4f^{14}5s\ ^2S_{1/2}$  levels in Pm-like Ir<sup>16+</sup> are very small, and the excitation energy of the  $4f^{14}5p\ ^2P_{1/2}$  is larger than the excitation energy of the  $4f^{14}5s\ ^2S_{1/2}$  by a factor of 12. All other levels listed in the third column of Table I belong to the  $4f^{13}5s5p$  and  $4f^{12}5s^25p$  configurations. First two excited states have transition frequencies to the ground state in the optical range. The energy differences between the  $4f^{13}5s\ ^3F_J$  (with  $J = 4$  and 3) levels and the  $4f^{14}\ ^1S_0$  level in Nd-like Ir<sup>17+</sup> is 4000-5000 cm<sup>-1</sup> according to COWAN code. However,

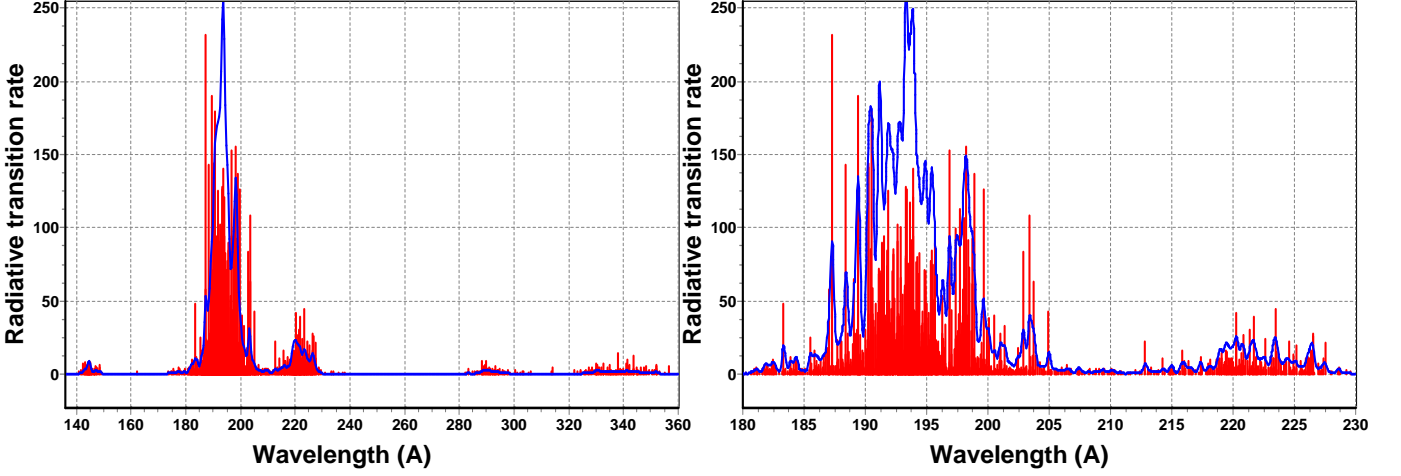


FIG. 2: Synthetic spectra (red) for the  $[4f^{14}5s + 4f^{13}5s5p + 4f^{12}5s5p^2] \leftrightarrow [4f^{14}5p + 4f^{13}5s^2 + 4f^{12}5s^25p]$  transitions (red) in Pm-like  $\text{Ir}^{16+}$  as a function of wavelength. Promethium is a rare earth element with  $Z = 61$ . A resolving power,  $R = E/\Delta E = 200$  and  $600$  (left and right) is assumed to produce a Gaussian profile (blue). The scale in the ordinate is in units of  $10^{10} \text{ s}^{-1}$ .

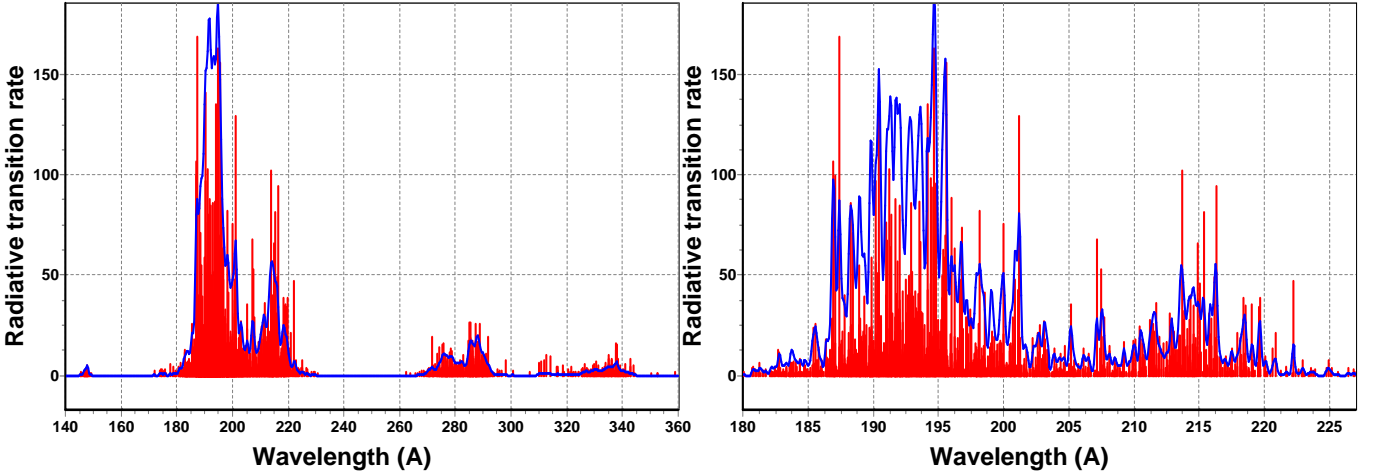


FIG. 3: Synthetic spectra (red) for the  $[4f^{14} + 4f^{13}5p + 4f^{12}5s^2 + 4f^{12}5p^2] \leftrightarrow [4f^{13}5s + 4f^{12}5s5p]$  transitions (red) in Nd-like  $\text{Ir}^{17+}$  as a function of wavelength. Neodymium is a rare earth element with  $Z = 60$ . A resolving power,  $R = E/\Delta E = 200$  and  $800$  (left and right) is assumed to produce a Gaussian profile (blue). The scale in the ordinate is in units of  $10^{10} \text{ s}^{-1}$ .

the uncertainties in these small energy differences may be particularly large. The excitation energies of the two other  $4f^{13}5s \ ^3F_2$  and  $4f^{13}5s \ ^1F_3$  levels are larger than the excitation energy of the  $4f^{13}5s \ ^3F_3$  level by a factor of 6-7 and the corresponding transition wavelengths to the ground state are in optical range. Almost all other levels listed in the column 6 of Table I belong to the  $4f^{12}5s^2$  and  $4f^{12}5s5p$  configurations. Only two levels belonging to the  $4f^{13}5p$  configuration have sufficiently low excitation energies to be included in our list of Nd-like  $\text{Ir}^{17+}$  levels in Table I.

The  $^2F$  ground state doublet splitting of the  $4f^{13}5s^2$  and  $4f^{13}$  configurations in Pm-like  $\text{Ir}^{16+}$  and Pr-like  $\text{Ir}^{18+}$  ions differs by only 2%. The transition from the next excited state of  $\text{Ir}^{18+}$  to the ground state is already in UV range. The first 25 low-lying levels of the Pr-like  $\text{Ir}^{18+}$  ion belong to the  $4f^{12}5s$  configuration, while the other 22 levels belong to the  $4f^{11}5s^2$  configuration.

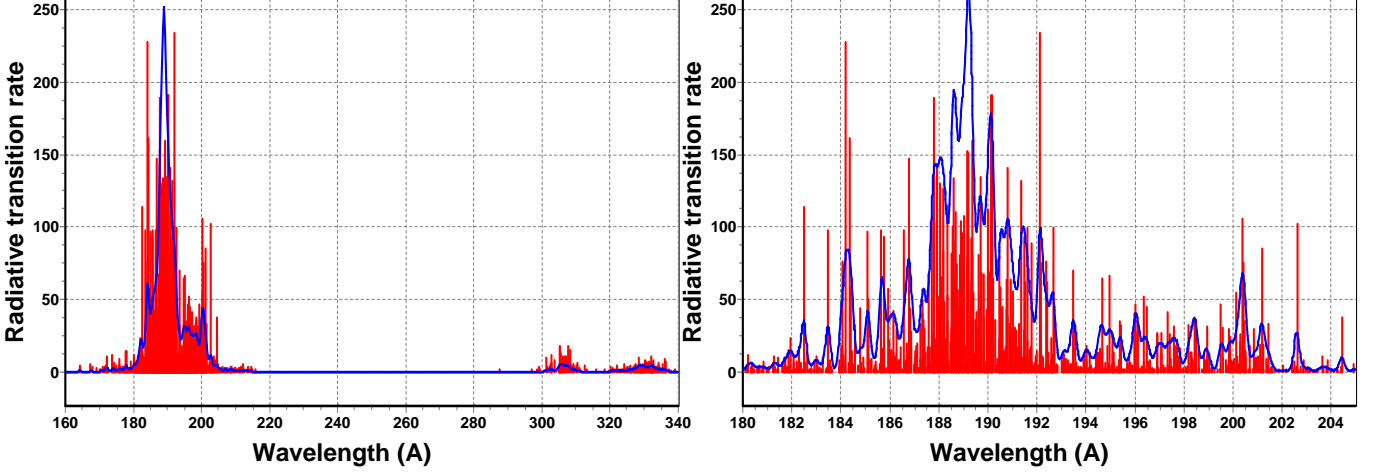


FIG. 4: Synthetic spectra (red) for the  $[4f^{13} + 4f^{12}5p + 4f^{11}5s^2] \leftrightarrow [4f^{12}5s + 4f^{11}5s5p]$  transitions (red) in Pr-like  $\text{Ir}^{18+}$  as a function of wavelength. Praseodymium (Pr) is a rare earth element with  $Z = 59$ . A resolving power,  $R = E/\Delta E = 200$  and 800 (left and right) is assumed to produce a Gaussian profile (blue). The scale in the ordinate is in units of  $10^{10} \text{ s}^{-1}$ .

#### IV. WAVELENGTHS, OSCILLATOR STRENGTHS, AND TRANSITION RATES

In Table II, we present selected set of our results for wavelengths ( $\lambda$  in Å), weighted oscillator strengths (gf), and weighted transition rates ( $gA_r$  in  $1/\text{s}$ ) for transitions between the  $4f$ -core-excited states. Only transition with the largest values of  $gA_r$  ( $gA_r > 10^{12} \text{ s}^{-1}$ ) are given.

We find that the  $4f^{12}5s^25p - 4f^{12}5s5p^2$  transitions have the largest values of  $gA_r$  for the Pm-like  $\text{Ir}^{16+}$ . This is expected since these arise from the one-electron electric-dipole  $5s - 5p$  transitions. The same type of the transitions are the strongest for the other two ions; the  $4f^{12}5s^2 - 4f^{12}5s5p$  and  $4f^{12}5s5p - 4f^{12}5p^2$  transitions for the Nd-like  $\text{Ir}^{17+}$  ion and  $4f^{11}5s^2 - 4f^{11}5s5p$  transitions in Pr-like  $\text{Ir}^{18+}$  ion, respectively. The transitions with the largest values of  $gA_r$  have wavelengths in the 187 - 200 Å range in  $\text{Ir}^{16+}$ , 187 - 214 Å range in  $\text{Ir}^{17+}$ , and 182 - 191 Å range in  $\text{Ir}^{18+}$ .

#### V. SYNTHETIC SPECTRA

Synthetic spectra for three Ir highly-charged ions are presented in Figs. 2, 3, and 4, respectively. We assume that spectral lines have the intensities proportional to the transition probabilities and are fitted with the Gaussian profile.

Synthetic spectra displayed in Figs. 2-4 are constructed from the following transitions:

- $\text{Ir}^{16+}$ :  $[4f^{14}5s + 4f^{13}5s5p + 4f^{12}5s5p^2] \leftrightarrow [4f^{14}5p + 4f^{13}5s^2 + 4f^{12}5s^25p]$ ,
- $\text{Ir}^{17+}$ :  $[4f^{14} + 4f^{13}5p + 4f^{12}5s^2] \leftrightarrow [4f^{13}5s + 4f^{12}5s5p]$ ,

- $\text{Ir}^{17+}$ :  $[4f^{13} + 4f^{12}5p + 4f^{11}5s^2] \leftrightarrow [4f^{12}5s + 4f^{11}5s5p]$ .

Every spectrum on the left panel of the figure includes about 2000 transitions with the values of  $gA_r > 10^{10} \text{ s}^{-1}$ . The synthetic spectra on the right panel include lines with the largest  $gA_r$  values. For example, the spectrum of  $\text{Ir}^{16+}$  displayed on the left panel of Fig. 2 includes the spectral region 140Å - 360Å. In the right panel of Fig. 2, we limit this region to 180Å - 230Å by neglecting the part of spectra with small intensity with the  $A_r$  value less than 10 in units of  $10^{10} \text{ s}^{-1}$ . The similar procedure was used for the other synthetic spectra.

Comparison of spectra at the right panels of Figs. 2, 3, and 4 shows the similarities including the main peak, some strong lines separate from the main peak and the second wide peak of small intensity. All strong lines are listed in Table II and Supplemental Material [5].

We note that present synthetic spectra do not take into account the population of states, and are meant to illustrate the distribution on the strongest lines. In typical EBIT conditions many of the states are barely populated, making the spectra significantly less dense [11, 12].

#### VI. MULTIPOLE TRANSITIONS, BRANCHING RATIOS, AND LIFETIMES

Wavelengths, transition rates, energies of the lower and upper level, lifetimes, and branching ratios from M1 and E1 transitions in Nd-, Pm-, and Pr-like Ir ions are presented in Table III. In order to determine the lifetimes listed in the last columns of Table III, we sum over all possible radiative transitions. The value of branching ratios for the particular transition is determined as a ra-

TABLE III: Wavelengths ( $\lambda$  in Å), transition rates ( $A_r$  in  $\text{s}^{-1}$ ), energies of the lower and upper level ( $\text{cm}^{-1}$ ), lifetimes ( $\tau$ ), and branching ratios (Branch. ratio) for M1 and E1 transitions in Pm-like  $\text{Ir}^{16+}$ , Nd-like  $\text{Ir}^{17+}$ , and Pr-like  $\text{Ir}^{18+}$  ions.

Conf.	Level	Conf.	Level	Energies in cm <sup>-1</sup>		λ	A <sub>r</sub>	Branch.	τ	
Upper Level		Lower level		Lower	Upper	Å	1/s	ratio		
Wavelengths, transition rates, lifetimes, and branching ratios from M1 and E1 transitions in Pm-like Ir <sup>16+</sup> ion										
4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>5/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>7/2</sub>	M1	0	25909	3860	2.69[+2]	1.00	3.71 ms
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> D <sub>7/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>7/2</sub>	E1	0	267942	373	1.24[+8]	0.97	7.80 ns
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> G <sub>11/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>7/2</sub>	E2	0	276214	362	1.19[+2]	1.00	8.37 ms
4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>2</sup> I <sub>13/2</sub>	4f <sup>12</sup> 5s <sup>2</sup> 5p	( <sup>3</sup> H) <sup>4</sup> G <sub>11/2</sub>	M1	276214	280512	23271	2.15[-1]	1.00	4.65 s
4f <sup>13</sup> 5s5p	( <sup>2</sup> F) <sup>4</sup> D <sub>7/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	( <sup>2</sup> F) <sup>2</sup> F <sub>7/2</sub>	E1	0	286286	349	3.54[+9]	0.98	0.278 ns
4f <sup>12</sup> 5s <sup>2</sup> 5p	(F) <sup>4</sup> D <sub>7/2</sub>	4f <sup>13</sup> 5s5p	(F) <sup>4</sup> D <sub>7/2</sub>	E1	267942	285301	5761	2.27[+0]	0.94	0.415 s
		4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>7/2</sub>	M1	0.000	285301	351	5.20[-2]	0.02	
		4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>5/2</sub>	M1	25.909	285301	385	8.49[-2]	0.04	
4f <sup>12</sup> 5s <sup>2</sup> 5p	(G) <sup>2</sup> H <sub>9/2</sub>	4f <sup>13</sup> 5s5p	(F) <sup>4</sup> D <sub>7/2</sub>	E1	267942	287909	5008	5.75[ 0]	0.92	0.161 s
		4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>5/2</sub>	E2	25909	287909	382	1.80[-1]	0.03	
		4f <sup>12</sup> 5s <sup>2</sup> 5p	(H) <sup>4</sup> G <sub>11/2</sub>	M1	276214	287909	23271	3.01[-1]	0.05	
4f <sup>13</sup> 5s5p	(F) <sup>4</sup> G <sub>9/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>7/2</sub>	E1	0	288623	346	4.69[+9]	1.00	0.213 ns
4f <sup>13</sup> 5s5p	(F) <sup>4</sup> F <sub>5/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>7/2</sub>	E1	0	289959	345	3.48[+9]	1.00	0.288 ns
4f <sup>13</sup> 5s5p	(F) <sup>4</sup> G <sub>5/2</sub>	4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>7/2</sub>	E1	0	297128	337	1.66[+9]	0.83	0.499 ns
		4f <sup>13</sup> 5s <sup>2</sup>	(F) <sup>2</sup> F <sub>5/2</sub>	E1	25909	297128	369	3.40[+8]	0.17	
Wavelengths, transition rates, lifetimes, and branching ratios from M1 and E1 transitions in Nd-like Ir <sup>17+</sup> ion										
4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>3</sub>	4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>4</sub>	M1	0	4236	23610	1.18[+0]	1.00	849 ms
4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>2</sub>	4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>3</sub>	M1	4236	26174	4558	2.26[+2]	1.00	4.42 ms
4f <sup>13</sup> 5s	(F) <sup>1</sup> F <sub>3</sub>	4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>4</sub>	M1	0	30606	3267	3.05[+2]	1.00	3.27 ms
4f <sup>12</sup> 5s <sup>2</sup>	(F) <sup>3</sup> F <sub>4</sub>	4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>3</sub>	E1	4236	42199	2634	6.51[+1]	0.97	14.9 ms
		4f <sup>13</sup> 5s	(F) <sup>1</sup> F <sub>3</sub>	E1	30606	42199	8626	1.79[+0]	0.03	
4f <sup>12</sup> 5s <sup>2</sup>	(H) <sup>3</sup> H <sub>5</sub>	4f <sup>12</sup> 5s <sup>2</sup>	(H) <sup>3</sup> H <sub>6</sub>	M1	33855	58261	4097	3.80[+2]	1.00	2.63 ms
4f <sup>12</sup> 5s <sup>2</sup>	(F) <sup>3</sup> F <sub>2</sub>	4f <sup>13</sup> 5s	(F) <sup>3</sup> F <sub>3</sub>	E1	4236	63696	1682	2.55[+2]	0.71	2.79 ms
		4f <sup>13</sup> 5s	(F) <sup>1</sup> F <sub>3</sub>	E1	30606	63696	3022	1.04[+2]	0.29	
4f <sup>12</sup> 5s5p	(H) <sup>5</sup> G <sub>6</sub>	4f <sup>12</sup> 5s <sup>2</sup>	(H) <sup>3</sup> H <sub>6</sub>	E1	33856	312026	359	2.65[+8]	0.97	3.68 ns
		4f <sup>12</sup> 5s <sup>2</sup>	(H) <sup>3</sup> H <sub>5</sub>	E1	58261	312026	394	6.72[+6]	0.03	
Wavelengths, transition rates, lifetimes, and branching ratios from M1 and E1 transitions in Pr-like Ir <sup>18+</sup> ion										
4f <sup>13</sup>	(F) <sup>2</sup> F <sub>5/2</sub>	4f <sup>13</sup>	(F) <sup>2</sup> F <sub>7/2</sub>	M1	0	26442	3782	2.86[+2]	1.00	3.49 ms
4f <sup>12</sup> 5s	(H) <sup>4</sup> H <sub>11/2</sub>	4f <sup>12</sup> 5s	(H) <sup>4</sup> H <sub>13/2</sub>	M1	60142	67687	13254	8.46[+0]	1.00	118 ms
4f <sup>12</sup> 5s	(F) <sup>4</sup> F <sub>9/2</sub>	4f <sup>13</sup>	(F) <sup>2</sup> F <sub>7/2</sub>	E1	0	70096	1427	5.92[+2]	1.00	0.169 ms
4f <sup>12</sup> 5s	(G) <sup>2</sup> G <sub>7/2</sub>	4f <sup>12</sup> 5s	(F) <sup>4</sup> F <sub>9/2</sub>	M1	70096	74664	21892	1.54[+0]	1.00	650 ms
4f <sup>12</sup> 5s	(H) <sup>4</sup> H <sub>9/2</sub>	4f <sup>12</sup> 5s	(H) <sup>4</sup> H <sub>11/2</sub>	M1	67687	87749	4985	2.81[+2]	1.00	3.55 ms
4f <sup>12</sup> 5s	(H) <sup>2</sup> H <sub>11/2</sub>	4f <sup>12</sup> 5s	(H) <sup>4</sup> H <sub>13/2</sub>	M1	60142	89858	3365	4.30[+2]	1.00	2.33 ms
4f <sup>12</sup> 5s	(F) <sup>4</sup> F <sub>5/2</sub>	4f <sup>12</sup> 5s	(G) <sup>2</sup> G <sub>7/2</sub>	M1	74664	92939	5472	4.23[+1]	1.00	23.7 ms
4f <sup>12</sup> 5s	(F) <sup>4</sup> F <sub>7/2</sub>	4f <sup>12</sup> 5s	(F) <sup>4</sup> F <sub>9/2</sub>	M1	70096	94507	4096	6.23[+1]	0.36	5.86 ms
4f <sup>12</sup> 5s	(G) <sup>2</sup> G <sub>9/2</sub>	4f <sup>12</sup> 5s	(G) <sup>2</sup> G <sub>7/2</sub>	M1	74664	94507	5039	1.01[+2]	0.59	5.88 ms
		4f <sup>12</sup> 5s	(F) <sup>4</sup> F <sub>9/2</sub>	M1	70096	98485	3522	1.67[+2]	0.98	

tio of the respective  $A_r$  values and the sum of all possible radiative transition rates that are used to determine the lifetimes. The number of contributing transitions increases significantly for higher levels. To save space, we only included the transitions that give the largest contributions to the lifetimes, and list additional transitions in the Supplemental Material [5].

We use atomic units (a.u.) to express all transition matrix elements throughout this section: the numerical values of the elementary charge,  $e$ , the reduced Planck

constant,  $\hbar = h/2\pi$ , and the electron mass,  $m_e$ , are set equal to 1. The atomic unit for electric-dipole matrix element is  $ea_0$ , where  $a_0$  is the Bohr radius.

The E1 and M1 transition probabilities  $A_r$  ( $\text{s}^{-1}$ ) are obtained in terms of line strengths  $S$  (a.u.) and wave-

TABLE IV: Energies (in  $\text{cm}^{-1}$ ) in Nd-like  $\text{Ir}^{17+}$  ions given relative to the  $4f^{13}5s^3F_4$  ground states. Comparison of the results calculated by the COWAN and RMBPT codes. The difference is given in percent in the last column.

Conf.	Level	Energy		Level	DIFF.
LSJ designations		$E^{\text{COWAN}}$	$E^{\text{RMBPT}}$	jj designations J	
$4f^{13}5s$	$(^2F)^3F_4$	0	0	$4f_{7/2}5s_{1/2}$	4
$4f^{13}5s$	$(^2F)^3F_3$	4236	4129	$4f_{5/2}5s_{1/2}$	3 2.5
$4f^{14}$	$(^1S)^1S_0$	5091	7055	$4f^{14}$	0 -38.5
$4f^{13}5s$	$(^2F)^3F_2$	26174	25447	$4f_{7/2}5s_{1/2}$	3 2.8
$4f^{13}5s$	$(^2F)^1F_3$	30606	30374	$4f_{5/2}5s_{1/2}$	4 0.8
$4f^{13}5p$	$(^2F)^3D_3$	319802	316065	$4f_{7/2}5p_{1/2}$	3 1.2
$4f^{13}5p$	$(^2F)^3G_4$	322623	319341	$4f_{7/2}5p_{1/2}$	4 1.0
$4f^{13}5p$	$(^2F)^3G_3$	346618	341890	$4f_{5/2}5p_{1/2}$	3 1.4
$4f^{13}5p$	$(^2F)^3F_2$	352344	348344	$4f_{5/2}5p_{1/2}$	2 1.1
$4f^{13}5p$	$(^2F)^3G_5$	482729	478806	$4f_{7/2}5p_{3/2}$	5 0.8
$4f^{13}5p$	$(^2F)^3D_2$	485701	481145	$4f_{7/2}5p_{3/2}$	2 0.9
$4f^{13}5p$	$(^2F)^1F_3$	491623	488430	$4f_{7/2}5p_{3/2}$	3 0.6
$4f^{13}5p$	$(^2F)^3F_4$	497788	494305	$4f_{7/2}5p_{3/2}$	4 0.7
$4f^{13}5p$	$(^2F)^3D_1$	502142	497907	$4f_{5/2}5p_{3/2}$	1 0.8
$4f^{13}5p$	$(^2F)^3G_4$	512504	507690	$4f_{5/2}5p_{3/2}$	4 0.9
$4f^{13}5p$	$(^2F)^3F_2$	519370	516116	$4f_{5/2}5p_{3/2}$	2 0.6
$4f^{13}5p$	$(^2F)^3F_3$	523054	518658	$4f_{5/2}5p_{3/2}$	3 0.8

TABLE V: Wavelengths ( $\lambda$  in  $\text{\AA}$ ), weighted oscillator strengths ( $gf$ ), weighted transition rates ( $gA_r$  in  $1/\text{s}$ ) for the  $4f^{14}5s - 4f^{14}5p_j$  transitions in Pm-like  $\text{Ir}^{16+}$ . Comparison of the results evaluated using the first-order RMBPT1, second-order RMBPT2, and the COWAN codes. Numbers in brackets represent powers of 10

	RMBPT1	RMBPT2	COWAN
$4f^{14}5s - 4f^{14}5p_{1/2}$ transition			
$\Delta E$ in $\text{cm}^{-1}$	312299	313974	309407
$\lambda$ in $\text{\AA}$	320.31	318.50	323.20
$gf$	0.5249	0.3809	0.3308
$gA_r$ in $1/\text{s}$	3.413[10]	2.522[10]	2.112[10]
$4f^{14}5s - 4f^{14}5p_{3/2}$ transition			
$\Delta E$ in $\text{cm}^{-1}$	469050	472710	469871
$\lambda$ in $\text{\AA}$	213.20	211.55	212.82
$gf$	1.6045	1.1754	1.4855
$gA_r$ in $1/\text{s}$	2.355[11]	1.752[11]	2.187[11]

lengths  $\lambda$  ( $\text{\AA}$ ) as

$$A(E1) = 2.02613 \times 10^{18} \frac{S(E1)}{(2J+1)\lambda^3}, \quad (1)$$

$$A(M1) = 2.69735 \times 10^{13} \frac{S(M1)}{(2J+1)\lambda^3}. \quad (2)$$

The line strengths  $S(E1)$  and  $S(M1)$  are obtained as squares of the corresponding E1 and M1 matrix elements.

In Table III, we include results for 8 selected electric-dipole and magnetic-multipole transitions that are the most important for the evaluation of the corresponding lifetimes in Pm-like  $\text{Ir}^{16+}$  ion. Results for 48 transitions

contributing to the lifetimes of 32 lowest levels are listed in the Supplemental Material [5]. Transitions with small branching ratios are omitted from the table.

The second excited state,  $4f^{14}5s^2S_{1/2}$ , is metastable with extremely long lifetime since the strongest possible decay channels are electric-octupole (E3) transition to the ground state, which is in optical range, and magnetic-quadrupole (M2) transition for the first excited level,  $4f^{13}5s^2^2F_{5/2}$ . These transitions are too weak to be estimated with the COWAN code, so we described such cases in text but omit from the Table III. There is only one such level for  $\text{Ir}^{16+}$  and  $\text{Ir}^{16+}$  ions and two levels for  $\text{Ir}^{17+}$  ion.

The lifetime of the first excited  $4f^{13}5s^2^2F_{5/2}$  state is equal to 3.71 ms with  $A_r$  equal to  $269 \text{ s}^{-1}$ . The lifetime of the third excited state is very short, 7.8 ns due to E1 allowed  $4f^{13}5s^2^2F_{7/2} - 4f^{13}5s5p^4D_{7/2}$  transition. The  $4f^{12}5s^25p^2I_{13/2}$  excited state is metastable with 4.65 s lifetime since the strongest transition is  $4f^{12}5s^25p^4G_{11/2} - 4f^{12}5s^25p^2I_{13/2}$  with small transition energy,  $4298 \text{ cm}^{-1}$ .

While some of the E1 transitions listed in Table III are strong allowed  $5s - 5p$  transitions, a number of E1 transitions are very weak since these are forbidden transitions with non-zero amplitude due to configuration mixing. For example, the  $A_r$  value of the  $4f^{13}5s^2^2F_{7/2} - 4f^{13}5s5p^4G_{9/2}$  transition is larger by nine orders of magnitude than  $4f^{13}5s5p^4D_{7/2} - 4f^{12}5s^25p^4D_{7/2}$  transition. In the first case, we have one-electron E1-allowed  $5s - 5p$  transition, while the second case is a strongly forbidden  $4f - 5s$  transition. The non-zero value of the  $4f^{13}5s5p^4D_{7/2} - 4f^{12}5s^25p^4D_{7/2}$  matrix element is due to mixing configurations.

In Table III, we include results for 10 selected electric-dipole and magnetic-multipole transitions that are the most important for the evaluation of the corresponding  $\text{Ir}^{17+}$  lifetimes. Results for 33 transitions contributing to the lifetimes of 13 lowest levels are listed in the Supplemental Material [5]. We also evaluated electric-quadrupole transitions, however, their contributions to lifetimes of levels given in Table III is negligible. Four of the transitions listed in Table III are M1 transitions between the states inside of the  $4f^{13}5s$  or  $4f^{12}5s^2$  configurations. While the  $4f^{13}5s - 4f^{12}5s^2$  transitions are E1-forbidden, their transition rates are non-zero due to mixing of the  $4f^{13}5s$  and the  $4f^{12}5s5p$  configurations. The lifetimes of most levels given in Table III are relatively long, since there are no allowed E1 transitions that may contribute to these lifetimes until the first level containing the  $5p$  electron. The resulting lifetime of the  $4f^{12}5s5p^5G_6$  level is very short, 3.68 ns due to the  $4f^{12}5s^2 - 4f^{12}5s5p$  E1 transitions.

Two  $\text{Ir}^{17+}$  levels,  $4f^{14}^1S_0$  and  $4f^{12}5s^2^3H_6$ , are extremely long lived making them potential candidates for the atomic clock scheme implementation. There is only extremely weak electric-octupole transition to the  $4f^{13}5s(^2F)^3F_3$  state contributing to  $^1S_0$  lifetime. The  $4f^{12}5s^2^3H_6$  lifetime is determined by the two the E3 and

TABLE VI: Comparison of the energies (in  $\text{cm}^{-1}$ ) in Nd-like  $\text{Ir}^{17+}$  ion given relative to the  $4f^{13}5s\ ^3F_4$  ground state obtained in different approximations [1, 3].

Conf.	Level	Energies in $\text{cm}^{-1}$		Diff. %	Energies in $\text{cm}^{-1}$		Diff. %
		COWAN	CI [1]		FSCC [3]	CIDFS [3]	
$4f^{13}5s$	$(^2F)^3F_4$	0	0				
$4f^{13}5s$	$(^2F)^3F_3$	4236	4838	12%	4662	4872	4%
$4f^{13}5s$	$(^2F)^3F_2$	26174	26272	0%	25156	25044	0%
$4f^{13}5s$	$(^2F)^1F_3$	30606	31492	3%	30197	30552	1%
$4f^{14}$	$(^1S)^1S_0$	5091	5055	-1%	13599	7025	-94%
$4f^{12}5s^2$	$(^3H)^3H_6$	33856	35285	4%	24221	29367	18%
$4f^{12}5s^2$	$(^3F)^3F_4$	42199	45214	7%	33545	38295	12%
$4f^{12}5s^2$	$(^3H)^3H_5$	58261	59727	2%	47683	52668	9%
$4f^{12}5s^2$	$(^3F)^3F_2$	63696	68538	7%	55007	60322	9%
$4f^{12}5s^2$	$(^3H)^1G_4$	66296	68885	4%	56217	60943	8%
$4f^{12}5s^2$	$(^3F)^3F_3$	68886	71917	4%	58806	63847	8%
$4f^{12}5s^2$	$(^3H)^3H_4$	89455	92224	3%	78534	82954	5%
$4f^{12}5s^2$	$(^3P)^1D_2$	91765	98067	6%	82422	88261	7%
$4f^{12}5s^2$	$(^1I)^1I_6$	101537	110065	8%	93867	101844	8%
$4f^{12}5s^2$	$(^3P)^3P_0$	101073	110717	9%	94012	99617	6%
$4f^{12}5s^2$	$(^3P)^3P_1$	107843	116372	7%	99416	105989	6%
$4f^{12}5s^2$	$(^1D)^3P_2$	117322			107489	113272	5%
$4f^{12}5s^2$	$(^1S)^1S_0$	178055			174893	185757	6%

one M2 channels:  $4f^{13}5s\ ^3F_3 - 4f^{12}5s^2\ ^3H_6$ ,  $4f^{13}5s\ ^1F_3 - 4f^{12}5s^2\ ^3H_6$ , and  $4f^{13}5s\ ^3F_4 - 4f^{12}5s^2\ ^3H_6$ .

In Table III, we include results for 10 selected electric-dipole and magnetic-multipole transitions that are most important for the evaluation of the corresponding lifetimes in Pr-like  $\text{Ir}^{18+}$  ion. Results for 51 transitions contributing to the lifetimes of 29 lowest levels are listed in the Supplemental Material [5]. Almost all transitions in Table III are magnetic-dipole transitions. Only last two lines include E1 forbidden transitions between  $4f^{12}5s$  and  $4f^{11}5s^2$  configurations. List of levels for the Pr-like  $\text{Ir}^{18+}$  ion in Table I covers the energy interval from the ground state up to  $274768\text{ cm}^{-1}$ . The first level with  $5p$  electron ( $4f^{12}5p\ ^4G_{11/2}$  level) has energy equal to  $387658\text{ cm}^{-1}$ . As a result, there are no electric-dipole allowed transitions in Table III.

The only extremely long-lived metastable level in  $\text{Ir}^{18+}$  ion is  $4f^{12}5s\ ^4H_{13/2}$  third excited state with  $E = 60142\text{ cm}^{-1}$ . This state can only decay via very weak electric-octupole transition to the ground state, which is in UV range.

The next longest lifetime, 8100 s, is for the  $4f^{12}5s\ ^2I_{11/2}$  level due to very small,  $205\text{ cm}^{-1}$ , energy difference in the  $4f^{12}5s\ ^2I_{13/2} - 4f^{12}5s\ ^2I_{11/2}$  transition. The  $4f^{11}5s^2\ ^2I_{13/2}$  level has short lifetime due to contribution of two E1 transitions via level mixing with branching ratios equal to 62% and 38%.

Dominant contribution to the  $4f^{12}5s^4F_{9/2}$  lifetime is from E1-forbidden transition to the  $4f^{13}\ ^2F_{7/2}$  state which is non-zero due to the 5% mixing between  $4f^{13}$  and  $4f^{12}5p$  configurations.

We did not find any theoretical or experimental results

to compare with our  $A_r$  and  $\tau$  values for the low-lying states listed in Table III.

## VII. COMPARISONS, UNCERTAINTY ESTIMATES, AND CONCLUSION

In Table IV, we compare energies in Nd-like  $\text{Ir}^{17+}$  ion calculated using the COWAN and RMBPT codes. Details of the RMBPT code for the hole-particle systems were presented by Safronova et. al. [13]. We use a complete set of Dirac-Fock (DF) wave functions on a nonlinear grid generated using B-splines [14] constrained to a spherical cavity. The basis set consists of 50 splines of order 9 for each value of the relativistic angular quantum number  $\kappa$ . The starting point for the RMBPT code is the *frozen core* DF approximation. We use second-order RMBPT to determine energies of the  $4f^{13}5s$  states relatively to the  $4f^{14}$  state in Nd-like  $\text{Ir}^{17+}$  ion.

The  $jj$  designation ( $4f_{7/2}5s_{1/2}$  for example) listed in Table IV means that we consider the system with  $4f_{7/2}$  hole in  $4f^{14}$  core and the  $5s_{1/2}$  particle. The  $LS$  designation are given in columns “1” and “2” of Table IV. The results with the same configuration and  $J$  are compared. The difference of RMBPT and COWAN data given in the last column of Table IV is less than 1% for most levels. The difference exceeds 3% only for  $4f^{14}$  level. This is the only level in the table that has a different number of  $4f$  electrons in comparison with the ground state. The correlation correction is very large for the  $4f$  state leading to this difference. For example, the calculation of the  $4f_{7/2}5s_{1/2}\ J = 4$  ground state energy gives  $5447\text{ cm}^{-1}$  in lowest order DF approximation, while the second order



TABLE VII: Comparison of the present results with theoretical [1, 3] and experimental [3] transition energies (in  $\text{cm}^{-1}$ ) for M1 transitions in Nd-like  $\text{Ir}^{17+}$  ion. Differences between experimental and theoretical results are given in per cent for all theoretical values.

Conf.	Transition	Energy Expt. [3]	Energy COWAN	Diff. %	Energy CI [1]	Diff. %	Energy FSCC [3]	Diff. %	Energy CIDFS [3]	Diff. %
$4f^{13}5s$	$^3F_2 - ^3F_3$	20710.83	21938	-6%	21434	-3%	20494	1%	20172	3%
$4f^{12}5s^2$	$^3H_4 - ^1G_4$	22430.03	23159	-3%	23339	-4%	22317	1%	22011	2%
$4f^{12}5s^2$	$^1G_4 - ^3F_4$	22948.54	24097	-5%	23671	-3%	22672	1%	22648	1%
$4f^{12}5s^2$	$^1D_2 - ^3F_3$	23162.84	22879	1%	26150	-13%	23616	-2%	24414	-5%
$4f^{12}5s^2$	$^3H_5 - ^3H_6$	23639.87	24405	-3%	24442	-3%	23462	1%	23301	1%
$4f^{12}5s^2$	$^3F_3 - ^3F_4$	25514.56	26687	-5%	26703	-5%	25261	1%	25552	0%
$4f^{12}5s^2$	$^1D_2 - ^3F_2$	27387.06	28069	-2%	29529	-8%	27415	0%	27939	-2%
$4f^{13}5s$	$^1F_3 - ^3F_4$	30358.45	30606	-1%	31492	-4%	30197	1%	30552	-1%
$4f^{12}5s^2$	$^3H_4 - ^3H_5$	30797.17	31194	-1%	32497	-6%	30851	0%	30286	2%

value is almost five times larger,  $-23997 \text{ cm}^{-1}$ . Adding the  $4577 \text{ cm}^{-1}$  QED and  $6888 \text{ cm}^{-1}$  Breit corrections gives  $-7055 \text{ cm}^{-1}$  relative to the frozen-core  $4f^{14}$  level.

In Table V, we compare wavelengths, weighted oscillator strengths, and weighted transition rates for the  $4f^{14}5s - 4f^{14}5p$  transitions in Pm-like  $\text{Ir}^{16+}$  evaluated using the first-order RMBPT1, second-order RMBPT2 [13], and the COWAN codes. COWAN code energy values are in somewhat better agreement with the first-order RMBPT results. The difference of RMBPT and COWAN code energies and wavelength is small, 0.18 % - 1.5 %, for wavelengths and energies of the  $4f^{14}5s - 4f^{14}5p$ .

The differences are larger, 7 % - 27 %, for the oscillator strength and transition rates. We find large effects of the second order corrections for these properties leading to larger differences in the results. In summary, the second-order correlation corrections are very important for accurate determination of the oscillator strengths and transition rates.

Energies (in  $\text{cm}^{-1}$ ) in Nd-like  $\text{Ir}^{17+}$  ion relative to the  $4f^{13}5s \ ^3F_4$  ground state obtained by the COWAN code are compared with results from Ref. [1] and [3] in Table VI. Results in [1] were obtained using configuration-interaction (CI) approach. Results in [3] were obtained using multireference Fock space coupled cluster (FSCC) method and configuration-interaction-Dirac-Fock-Sturmian (CIDFS) method. COWAN results were also presented in [3]. The largest difference (12%) between the COWAN and CI [1] results is for the first excited state. For other levels, the difference is about 3-4%. The largest difference (94%) between results in Ref. [3], evaluated by FSCC and CIDFS methods are for the  $4f^{14} \ ^1S_0$  level. For other levels, the difference is about 5-9%.

Comparison of the present results with theoretical [1, 3] and experimental [3] transition energies (in  $\text{cm}^{-1}$ ) for M1 transitions in Nd-like  $\text{Ir}^{17+}$  ion are given in Table VII. In [3], improved accuracy measurements were performed for the  $\text{Ir}^{17+}$  transitions by repeating a calibration-measurement-calibration cycle five times at one grating

position. Each cycle takes 15-30 min. The transition energy was determined by averaging the line centroids in typically 30 of such acquired spectra. Results are given for the M1 transitions between the states of the  $4f^{13}5s$  and  $4f^{12}5s^2$  configurations. The differences between the experimental results and theoretical values obtained by the COWAN code, CI [1], FSCC and CIDFS [3] are given in percent. The largest difference between the experimental values [3] and the COWAN code results is 6%, while the difference is twice as large for CI values [1]. The differences between the FSCC [3] and CIDFS [3] results and experiment [3] are 0-2% and 0-5%, respectively.

In summary, we carried out a systematic study of excitation energies, wavelengths, oscillator strengths, and transition rates in  $\text{Ir}^{16+}$ ,  $\text{Ir}^{17+}$ , and  $\text{Ir}^{18+}$  ions. Synthetic spectra are constructed for all three ions, with the strongest line regions presented in more detailed on a separate panel. Metastable states and importance of the M1 transitions for the determination of the lifetimes are discussed. Comparison of the energy values with other theoretical predictions is given. Transition wavelengths are compared with the experiment [3] and other theory. We did not find any other theoretical results of oscillator strength and transitions rates in the ions considered in the present study. We believe that our predictions will be useful for planning and analyzing future experiments with highly-charged ions.

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